A NUMERICAL AND SYMBOLICAL APPROXIMATION OF THE NONLINEAR ANDERSON MODEL

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Abstract. A modified perturbation theory in the strength of the nonlinear term is used to solve the Nonlinear Schrödinger Equation with a random potential. It is demonstrated that in some cases it is more efficient than other methods. Moreover we obtain error estimates. This approach can be useful for the solution of other nonlinear differential equations of physical relevance.

1. Introduction

We consider the problem of dynamical localization of waves in a Nonlinear Schrödinger Equation (NLSE) [1] with a random potential term on a lattice:

$$i\partial_t\psi = -J\left[\psi\left(x+1\right)+\psi\left(x-1\right)\right]+\varepsilon_x\psi+\beta\left|\psi\right|^2\psi, \tag{1.1}$$

where $\psi = \psi\left(x,t\right)$, $x\in\mathbb{Z}$; and $\{\varepsilon_x\}$ is a collection of i.i.d. random variables uniformly distributed in the interval $\left[-\frac{W}{2},\frac{W}{2}\right]$.

The NLSE was derived for a variety of physical systems under some approximations. It was derived in classical optics where ψ is the electric field by expanding the index of refraction in powers of the electric field keeping only the leading nonlinear term [2]. For Bose-Einstein Condensates (BEC), the NLSE is a mean field approximation where the term proportional to the density $\beta|\psi|^2$ approximates the interaction between the atoms. In this field the NLSE is known as the Gross-Pitaevskii Equation (GPE) [3, 4, 5, 6, 7, 8]. Recently, it was rigorously established, for a large variety of interactions and of physical conditions, that the NLSE (or the GPE) is exact in the thermodynamic limit [9, 10]. Generalized mean field theories, in which several mean-fields are used, were recently developed [11, 12]. In the absence of randomness (1.1) is completely integrable. For repulsive nonlinearity ($\beta>0$) an initially localized wavepacket spreads, while for attractive nonlinearity ($\beta<0$) solitons are found typically [1].

For $\beta=0$ this equation reduces to the Anderson model [13],

$$i\partial_t\psi = -J\left[\psi\left(x+1\right)+\psi\left(x-1\right)\right]+\varepsilon_x\psi. \tag{1.2}$$

It is well known that in 1D in the presence of a random potential with probability one all the states are exponentially localized [13, 14, 15, 16]. Consequently, diffusion is suppressed and in particular a wavepacket that is initially localized will not spread to infinity. This has been very recently extended to the many-body particle system [17, 18, 19]. This is the phenomenon of Anderson localization. In 2D it is known heuristically from the scaling theory of localization [20, 15] that all the states are localized, while in higher dimensions there is a mobility edge that separates localized

Date: December 19, 2009.

Key words and phrases. Anderson localization, NLSE, random potential, nonlinear Schrodinger, dynamical localization, diffusion, sub-diffusion.

and extended states. This problem is relevant for experiments in nonlinear optics, for example disordered photonic lattices [21], where Anderson localization was found in presence of nonlinear effects as well as experiments on BECs in disordered optical lattices [22, 23, 24, 25, 26, 27, 28, 29, 30]. The interplay between disorder and nonlinear effects leads to new interesting physics [28, 29, 31, 32, 33, 34]. In spite of the extensive research, many fundamental problems are still open, and in particular, it is not clear whether in one dimension (1D) Anderson localization can survive the effects of nonlinearities (see however [35, 36]).

A natural question is whether a wave packet that is initially localized in space will indefinitely spread for dynamics controlled by (1.1). A simple argument indicates that spreading will be suppressed by randomness. If unlimited spreading takes place the amplitude of the wave function will decay since the L^2 norm is conserved. Consequently, the nonlinear term will become negligible and Anderson localization will take place as a result of the randomness. Contrary to this intuition, based on the smallness of the nonlinear term resulting from the spread of the wave function, it is claimed that for the kicked-rotor a nonlinear term leads to delocalization if it is strong enough [37]. It is also argued that the same mechanism results in delocalization for the model (1.1) with sufficiently large β, while, for weak nonlinearity, localization takes place [37, 38]. Therefore, it is predicted in that work that there is a critical value of β that separates the occurrence of localized and extended states. However, if one applies the arguments of [37, 38] to a variant of (1.1), results that contradict numerical solutions are found [39, 40]. Recently, it was rigorously shown that the initial wavepacket cannot spread so that its amplitude vanishes at infinite time, at least for large enough β [41]. It does not contradict spreading of a fraction of the wavefunction. Indeed, subdiffusion was found in numerical experiments [37, 41, 42]. In different works [42, 43, 44] sub-diffusion was reported for all values of β. It was also argued that nonlinearity may enhance discrete breathers [33, 34]. In conclusion, it is *not* clear what is the long time behavior of a wave packet that is initially localized, if both nonlinearity and disorder are present. The major difficulty in numerical resolution of this question is integration of (1.1) to large time. Most researchers who run numerical simulation use a split-step method for integration, however it is impossible to achieve convergence for large times, and therefore some heuristic arguments assuming that the numerical errors do not affect the results qualitatively, are utilized [37, 43]. However it is unclear whether those arguments apply to (1.1). The motivation of the current work is to propose a numerical scheme based on a modified perturbation theory developed in [45, 46] which will allow integration of (1.1) and similar equations up to large times and with some control of the error based on the form of the remainder term obtained in [46].

The advantage of the perturbative method is that it provides an estimate of the error while there is no such estimate in the split-step method. Moreover the error in the split-step method is expected to proliferate as a result of the nonlinearity.

In Section 2 we briefly review the perturbation theory developed in [46]. In Section 3 we explain the numerical scheme used to compute the different orders in the perturbation theory. In Section 4 we show how the error of the perturbation theory could be controlled. In Section 5 we present the comparison between the perturbation theory and an exact integration. The results are summarized in Section 6 and open problems are listed there.

In summary, this work demonstrates a numerical implementation of the perturbation theory for (1.1) in powers of β which was described in [46], and evaluates its possible use.

2. The perturbation theory

Our goal is to analyze the nonlinear Schrödinger equation (1.1) that could be written in the form

$$i\partial_t\psi = H_0\psi + \beta\left|\psi\right|^2\psi \tag{2.1}$$

where H_0 is the Anderson Hamiltonian,

$$H_0\psi\left(x\right) = -J\left[\psi\left(x+1\right)+\psi\left(x-1\right)\right]+\varepsilon_x\psi\left(x\right). \tag{2.2}$$

The wavefunction can be expanded using the eigenstates, $u_m\left(x\right)$, and eigenvalues, E_m, of H_0 as

$$\psi\left(x,t\right) = \sum_m c_m\left(t\right)e^{-iE_mt}u_m\left(x\right). \tag{2.3}$$

For the nonlinear equation the dependence of the expansion coefficients, $c_n\left(t\right)$, is found by inserting this expansion into (2.1), resulting in

$$i\partial_t c_n = \beta\sum_{m_1,m_2,m_3} V_n^{m_1m_2m_3}c_{m_1}^*c_{m_2}c_{m_3}e^{i\left(E_n+E_{m_1}-E_{m_2}-E_{m_3}\right)t} \tag{2.4}$$

where $V_n^{m_1m_2m_3}$ is an overlap sum

$$V_n^{m_1m_2m_3} = \sum_x u_n\left(x\right)u_{m_1}\left(x\right)u_{m_2}\left(x\right)u_{m_3}\left(x\right). \tag{2.5}$$

Our objective is to develop a perturbation expansion of the $c_m\left(t\right)$ in powers of β and to calculate them order by order in β. The required expansion is

$$c_n\left(t\right) = c_n^{(0)}+\beta c_n^{(1)}+\beta^2c_n^{(2)}+\cdots+\beta^Nc_n^{(N)}+Q_n, \tag{2.6}$$

where the expansion is till order N and Q_n is the remainder term (note here Q_n differs from one defined in [46]). We will assume the initial condition

$$c_n\left(t=0\right) = \delta_{n0}. \tag{2.7}$$

The equations for the two leading orders are presented in what follows. The leading order is

$$c_n^{(0)} = \delta_{n0}. \tag{2.8}$$

And the first order is

$$c_n^{(1)} = V_n^{000}\left(\frac{1-e^{i(E_n-E_0)t}}{E_n-E_0}\right). \tag{2.9}$$

We notice that divergence of this expansion for any value of β may result from three major problems: the secular terms problem, the entropy problem (i.e., factorial proliferation of terms), and the small denominators problem. In this paper we will not discuss the entropy problem and the problem of small denominators, since it was done in detail in [46]. We first show how to derive the equations for $c_n\left(t\right)$ where the secular terms are eliminated. To achieve this we replace the ansatz (2.3) by

$$\psi(x,t) = \sum_n c_n(t)\, e^{-iE'_n t} u_n(x) \tag{2.10}$$

where

$$E'_n \equiv E_n^{(0)} + \beta E_n^{(1)} + \beta^2 E_n^{(2)} + \cdots \tag{2.11}$$

and $E_n^{(0)}$ are the eigenvalues of H_0. We will dub E'_n the renormalized energies. The new equation for the c_n is given by

$$i\partial_t c_n = \left(E_n^{(0)} - E'_n\right) c_n + \beta \sum_{m_1 m_2 m_3} V_n^{m_1 m_2 m_3} c^*_{m_1} c_{m_2} c_{m_3} e^{i\left(E'_n + E'_{m_1} - E'_{m_2} - E'_{m_3}\right)t}. \tag{2.12}$$

Inserting expansions (2.6) and (2.11) into (2.12) and comparing the powers of β *without expanding the exponent* in β, produces the following equation for the $k-th$ order

$$\begin{aligned} i\partial_t c_n^{(k)} = &-\sum_{s=0}^{k-1} E_n^{(k-s)} c_n^{(s)} + \\ &+ \sum_{m_1 m_2 m_3} V_n^{m_1 m_2 m_3} \left[\sum_{r=0}^{k-1} \sum_{s=0}^{k-1-r} \sum_{l=0}^{k-1-r-s} c_{m_1}^{(r)*} c_{m_2}^{(s)} c_{m_3}^{(l)}\right] e^{i\left(E'_n + E'_{m_1} - E'_{m_2} - E'_{m_3}\right)t}. \end{aligned} \tag{2.13}$$

Note that the exponent is of order $O(1)$ in β, and therefore we may choose not to expand it in powers of β. However, it results in an expansion where both $E_m^{(l)}$ and $c_n^{(k)}$ depend on β. For the expansion (2.6) to be valid, both $E_m^{(l)}$ and $c_n^{(k)}$ should be $O(1)$ in β, this is satisfied, since the RHS of (2.13) contains only $c_n^{(r)}$ such that $r < k$. Namely, this equation gives each order in terms of the lower ones, with the initial condition of $c_n^{(0)}(t) = \delta_{n0}$. Solution of k equations (2.13) gives the solution of the differential equation (2.12) to order k, while the higher order terms which are obtained from this equation are meaningless (see Appendix for the reasoning). Since, the exponent in (2.13) is of order $O(1)$ in β we can select its argument to be of any order in β. However, for the removal of the secular terms, as will be explained bellow, it is instructive to set the order of the argument to be $k-1$, as the higher orders were not calculated at this stage. Secular terms are created when there are time independent terms in the RHS of the equation above. We eliminate those terms by using the first two terms in the first summation on the RHS. We make use of the fact that $c_n^{(0)} = \delta_{n0}$ and $c_n^{(1)}$ can be easily determined (see (2.16,2.15)), and used to calculate $E_{n=0}^{(k)}$ and $E_{n\neq 0}^{(k-1)}$ that eliminate the secular terms in the equation for $c_n^{(k)}$, that is

$$E_n^{(k)} c_n^{(0)} + E_n^{(k-1)} c_n^{(1)} = E_n^{(k)} \delta_{n0} + E_n^{(k-1)} (1 - \delta_{n0}) \frac{V_n^{000}}{E'_n - E'_0}, \tag{2.14}$$

where only the time-independent part of $c_n^{(1)}$ was used. In other words, we choose $E_n^{(k)}$ and $E_{n\neq 0}^{(k-1)}$ so that the time-independent terms on the RHS of (2.13) are eliminated. $E_0^{(k)}$ will eliminate all secular terms with $n = 0$, and $E_n^{(k-1)}$ will

eliminate all secular terms with $n \neq 0$. In the following, we will demonstrate this procedure for the first order.

In the first order of the expansion in β we obtain

$$\begin{aligned} i\partial_t c_n^{(1)} &= -E_n^{(1)} c_n^{(0)} + \sum_{m_1 m_2 m_3} V_n^{m_1 m_2 m_3} c_{m_1}^{*(0)} c_{m_2}^{(0)} c_{m_3}^{(0)} e^{i\left(E'_n + E'_{m_1} - E'_{m_2} - E'_{m_3}\right)t} \\ &= -E_n^{(1)} \delta_{n0} + V_n^{000} e^{i\left(E'_n - E'_0\right)t}. \end{aligned} \tag{2.15}$$

For $n = 0$ the equation produces a secular term

$$\begin{aligned} i\partial_t c_0^{(1)} &= -E_0^{(1)} + V_0^{000} \\ c_0^{(1)} &= it \cdot \left(E_0^{(1)} - V_0^{000}\right). \end{aligned} \tag{2.16}$$

Setting

$$E_0^{(1)} = V_0^{000} \tag{2.17}$$

eliminates this secular term and gives

$$c_0^{(1)} = 0. \tag{2.18}$$

For $n \neq 0$ there are no secular terms in this order, therefore finally

$$c_n^{(1)} = (1 - \delta_{n0})\, V_n^{000} \left(\frac{1 - e^{i\left(E'_n - E'_0\right)t}}{E'_n - E'_0} \right), \tag{2.19}$$

where to this order $E'_n = E_n$ and $E'_0 = E_0$.

The higher order terms in the perturbation theory are given by recursive relations and due to the large number of terms which are involved will be calculated numerically.

3. The numerical method

In order to compute the various orders in the perturbation theory we use equation (2.13), which is a recursive equation of the orders. To compute order k we have to compute all $c_n^{(l)}$ and $E_n^{(l)}$ for $l \leq k-1$. The numerical calculation is done in two stages: at the first stage a symbolic calculation of the expressions of all the $c_n^{(l)}$ and $E_n^{(l)}$ is performed, this has a complexity of $O\left(e^{2k}\right)$, which is due to the increasing number of terms in each expression for $c_n^{(l)}$ (see [46]). This stage does not depend neither on the realization nor the nonlinearity strength, β. In the second stage realizations and β are chosen and $c_n^{(l)}$ and $E_n^{(l)}$ are calculated. This stage has a complexity of $O\left(e^{2k} \cdot L^k\right)$, where L is the dimension of the lattice. The computation of this stage could be fully parallelized.

When calculating $E_n^{(l)}$ we encounter self-consistent equations of the type

$$E_n^{'} = f_n\left(\left\{E_m^{'}\right\}\right), \tag{3.1}$$

where f is some function, for example for the second order

$$E'_n = E_n^{(0)} + \beta V_n^{n00}\left(2 - \delta_{n0}\right) - 3\beta^2 \delta_{n0} \sum_{m \neq 0} \frac{\left(V_m^{000}\right)^2}{E'_m - E'_0}. \tag{3.2}$$

Higher order equations are required in general. We solve those equations numerically by reinserting the LHS into the RHS, until a desired convergence is achieved.

The first iteration is done by setting $\beta = 0$ at the RHS. Basically, at each iteration an order of β is gained in the accuracy of the solution and since we need to know $E_n^{'}$ only to a desired order N (see Appendix), only a small number of iterations is needed. The $c_n^{(l)}$ are represented as vectors with elements $\left(c_{n,\omega_1}^{(l)}, c_{n,\omega_2}^{(l)}, \ldots\right)$ identified by frequencies such that terms with same frequencies are grouped together (by summing their amplitudes), namely, $c_{n,\omega_k}^{(l)} = \sum_j c_{n,\omega_k,j}^{(l)} e^{-i\omega_k t}$, where ω_k is a shared frequency. Due to the fact that most of the amplitudes are negligible, after grouping a thresholding step is done and terms which are smaller than 10^{-6} are eliminated. The error introduced by the tresholding can be easily controlled, since we know how many frequencies were left out. By having the vector of frequencies and their corresponding amplitudes we can calculate the perturbative solution at any time. Even after grouping and thresholding the number of frequencies is growing rapidly with the order of the expansion.

4. The remainder of the expansion

In order to control the solution we have to control, Q_n, the remainder of the expansion (2.6) that can be written in the form

$$c_n(t) = \tilde{c}_n + Q_n, \tag{4.1}$$

with

$$\tilde{c}_n = \sum_{l=0}^{N} \beta^l c_n^{(l)}. \tag{4.2}$$

It is useful to define

$$\tilde{\psi}(x,t) = \sum_m \tilde{c}_m u_m(x) e^{-iE_m^{'}t} \tag{4.3}$$

and

$$\tilde{Q}_n = Q_n e^{-iE_n^{'}t}. \tag{4.4}$$

Substituting (4.1) in (2.12) leads to the following equation for the remainder which is expressed in terms of (4.2), (4.3) and (4.4),

$$i\partial_t \tilde{Q}_n = W_n(t) + \sum_m M_{nm}(t)\tilde{Q}_m + \sum_m \bar{M}_{nm}(t)\tilde{Q}_m^* + F\left(\tilde{Q}\right) \tag{4.5}$$

where

$$\begin{aligned} W_n(t) &= \left(E_n^{(0)} - E_n^{'}\right)\tilde{c}_n e^{-iE_n^{'}t} - i\left(\partial_t \tilde{c}_n\right)e^{-iE_n^{'}t} \\ &+ \beta\sum_x u_n(x)\left|\tilde{\psi}(x)\right|^2\tilde{\psi}(x) \end{aligned} \tag{4.6}$$

is the inhomogeneous term,

$$M_{nm}(t) = E_n^{(0)}\delta_{nm} + 2\beta\sum_x u_n(x)\left|\tilde{\psi}(x)\right|^2 u_m(x) \tag{4.7}$$

and

$$\bar{M}_{nm}(t) = \beta\sum_x u_n(x)\left(\tilde{\psi}(x)\right)^2 u_m(x). \tag{4.8}$$

determine the linear terms, while the nonlinear term is,

$$
\begin{aligned}
F\left(\bar{Q}\right) &= \beta\sum_{x} u_n\left(x\right)\tilde{\psi}^{*}\left(x\right)\left(\sum_{m}\tilde{Q}_m u_m\left(x\right)\right)^2 \\
&+ 2\beta\sum_{x} u_n\left(x\right)\tilde{\psi}\left(x\right)\left|\sum_{m}\tilde{Q}_m u_m\left(x\right)\right|^2 \\
&+ \beta\sum_{x} u_n\left(x\right)\left|\sum_{m}\tilde{Q}_m u_m\left(x\right)\right|^2\left(\sum_{m}\tilde{Q}_m u_m\left(x\right)\right).
\end{aligned}
\tag{4.9}
$$

The linear part of (4.5) is given by

$$
i\partial_t\tilde{Q}_n^{lin} = W_n\left(t\right) + \sum_{m} M_{nm}\left(t\right)\tilde{Q}_m^{lin} + \sum_{m}\bar{M}_{nm}\left(t\right)\left(\tilde{Q}_m^{lin}\right)^{*}. \tag{4.10}
$$

Using a bootstrap argument, which utilizes the continuity of (4.5) and smallness of the linear part of (4.10) one can show [46] that until some time t_* , the dynamics of (4.5) is governed by the linear part and the remainder is bounded by,

$$
\left|Q_n\left(t\right)\right| \leq A\cdot t\cdot e^{-\gamma|n|}, \tag{4.11}
$$

where γ is the inverse localization length. Therefore to estimate the remainder we can integrate (4.10) instead of (4.5) at least up to t_*. It is useful to integrate up to some large time, $t \ll t_*$, and then to extrapolate using the linear bound (4.11) up to t_*. In the next section it will be proposed how to determine t_* in practice.

5. Results

In this section it will be demonstrated, how the numerical scheme for calculations in the framework of the perturbation theory, is implemented in practice. Some results will be compared with an exact numerical solution of the original equation (1.1).

For this purpose we have calculated numerically all the $c_n^{(l)}$ and $E_n^{'}$ for $l \leq 4$ for a certain realization of the random potential. To compare perturbation theory results to the exact results, we compute their Fourier transform for different orders of expansion. On Fig. 5.1 we see the Fourier transform of $\bar{c}_0$, $\bar{c}_1$ and $\bar{c}_9$ (see (4.2)) compared to the Fourier transform of an exact (numerical) solution, c_n, calculated using a split-step method. We notice a reasonable agreement of the perturbation theory with an exact solution for $\bar{c}_0$, $\bar{c}_1$ and a disagreement for $\bar{c}_9$. By plotting $Q_n^{lin}\left(t\right)$ for all n with the same scale (on the same axis) in Fig. 5.2, we see that there are modes (on Fig. 5.2 there are two of them) which contribute to most of the discrepancy in the perturbation theory calculation, since if $Q_n^{lin}\left(t\right)$ is large the bound on $Q_n\left(t\right)$ is also large.

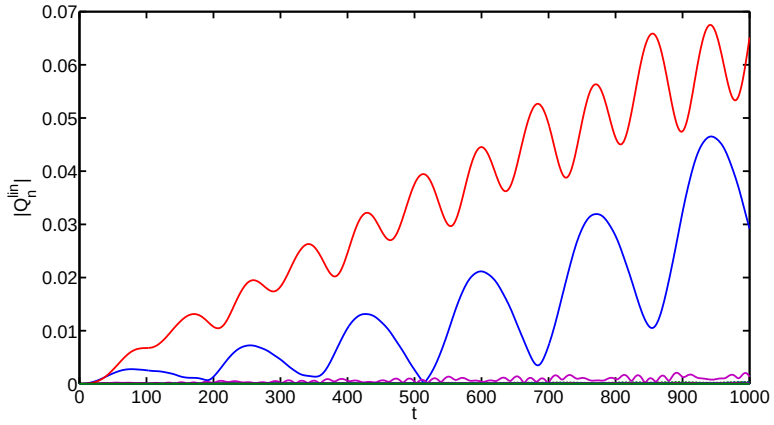

Figure 5.2: Q_n^{lin} as a function of time in the 4th order in β for all n's of the lattice (total 128 lines). The two lines that are far above the rest (which are barely visible) correspond to the resonant modes, $n = 4, 9$. The parameters are: $\beta = 0.0774$, $W = 4$, $J = 1$.

We will call those modes resonant modes. In Fig. 5.3 we compare a norm of Q_n, calculated with the resonant modes,

$$\|Q\|_2 = \left(\sum_m |Q_m|^2\right)^{1/2}, \tag{5.1}$$

and without them $\|Q'\|_2$.

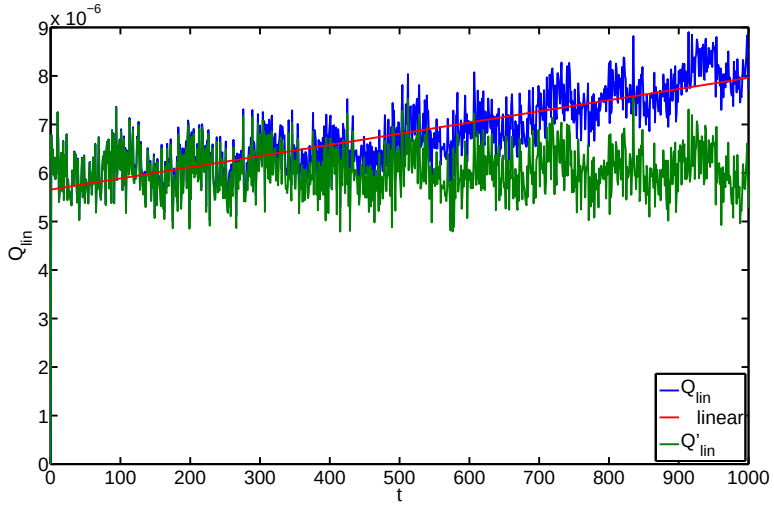

Figure 5.3: $\|Q\|_2$ (dashed blue) and $\|Q'\|_2$ (solid green) as a function of time. The straight line is a linear fit to $\|Q\|_2$. The parameters are: 4th order, $\beta = 0.01$, $W = 4$, $J = 1$. The linear fit is: $\|Q\|_2(t) = 2.3 \times 10^{-9} \cdot t + 5.7 \times 10^{-6}$.

It is found that indeed the $\|Q\|_2$ grows linearly with time as expected from (4.11). Actually, this is the way a bound on the resonant terms is expected to behave [46]. It is evident that by excluding the resonant modes the discrepancy between the perturbation theory and exact results is much lower. The reason why the perturbation theory fails for the resonant modes is that they correspond to a quasi-degeneracy, namely, when $E'_n \approx E'_0$, and the overlap $\left|V_n^{000}\right|$ is not sufficiently small. A natural way to quantify the resonance condition is to use (compare to Eq.(5) of [43]),

$$R_n^{-1} \equiv \left| \frac{V_n^{000}}{E'_n - E'_0} \right| . \tag{5.2}$$

The resonant modes produce substantially higher values of R_n^{-1} compared to any other modes as demonstrated in Fig. 5.4.

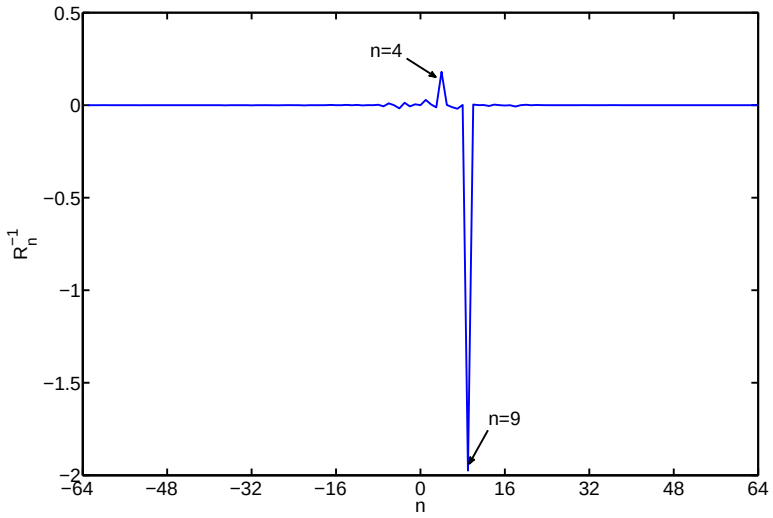

Figure 5.4: R_n^{-1} as a function of n

One way to deal with this problem is by using a degenerate perturbation theory. However it is an open question how to implement it for a nonlinear problem, that should be left for further studies.

At the end of the last section we have claimed that for some time, t_*, the linear part of (4.5) dominates over the nonlinear part given that the linear part is sufficiently small. In Fig. 5.5 we present a comparison between the solution of the linear equation (4.10) and Q_{ex}, the solution of (4.5). It is clear that until $\|Q_{lin}\|_2 \sim 0.1$ both the solutions are very close.

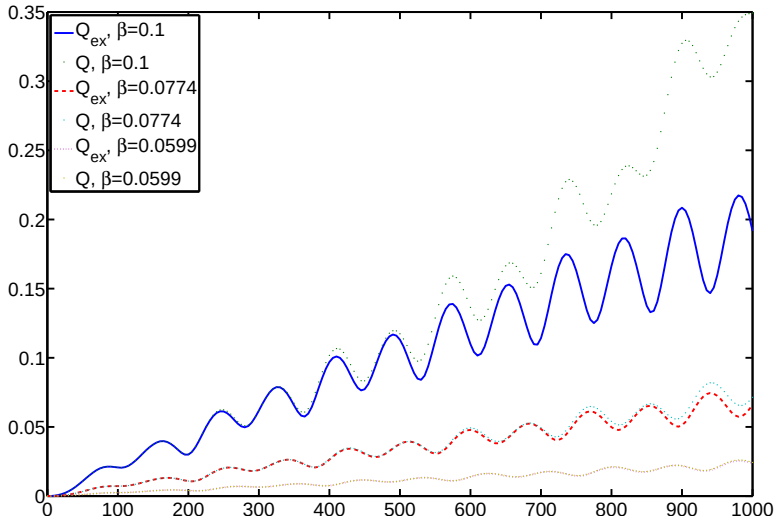

Figure 5.5: $\|Q_{ex}\|_2$ (lines) and $\|Q_{lin}\|_2$ (dotes) as a function of time, for various values of β (see legend). The perturbation expansion is up to fourth order in β.

We use this value to define t_*,

$$\|Q_{lin}(t_*)\|_2 = 0.1. \tag{5.3}$$

For small nonlinearity strength, β, t_* is very large and therefore the integration of (4.10) to t_* is very time consuming. We therefore use the bound (4.11) to extrapolate linearly from the time interval where (4.10) is solved to t_*. Practically, we have calculated the linear behavior of Q_{lin} like it was done in Fig. 5.3 than we found t_* from (5.3). In Fig. 5.6 we plot $\log_{10} t_*$ as a function of β^{-1} for different orders, while in Fig. 5.7 we compare the result found in 4-th order with $\left|Q_n^{lin}\right|$ of (5.3) is replaced by $\left|Q_n^{lin'}\right|$ (where the resonant terms are removed)

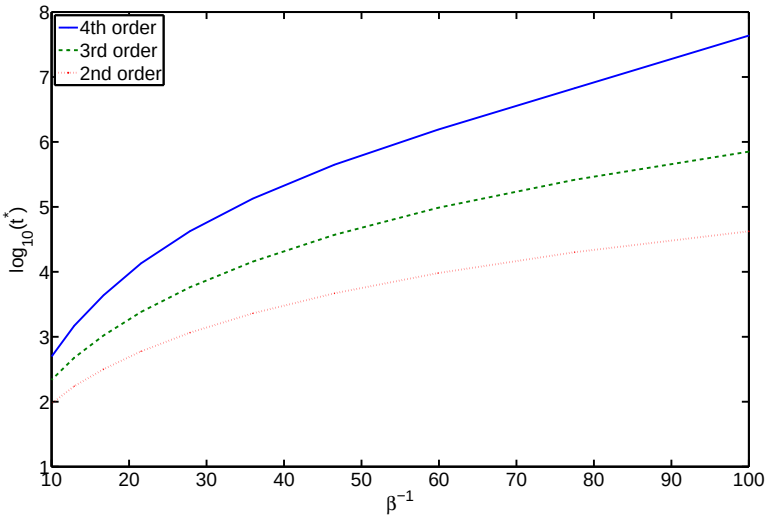

Figure 5.6: $\log_{10} t_*$ as a function of β^{-1} for different orders. 4th order (solid blue), 3rd order (dashed green) and 2nd order (dotted red). The parameters are: $W = 4$, $J = 1$.

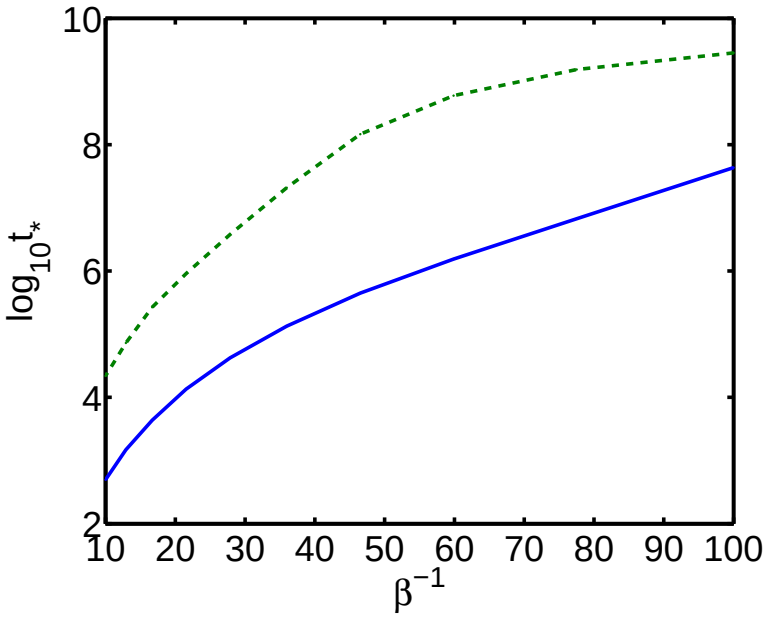

Figure 5.7: $\log_{10} t_*$ as a function of β^{-1} for the 4-th order.. Solid blue line is when t_* is calculated based on $\left|Q_n^{lin}\right|$ and dashed green line is when $\left|Q_n^{lin'}\right|$ is used instead. The parameters are: $W = 4$, $J = 1$.

A systematic improvement with the order of the perturbation theory is found. We notice that even with moderate nonlinearity strengths, namely, $\beta < 0.08$, one can achieve a good approximation of the solution up to very large times. In this way the perturbation theory combined with the solution of the linear equation (4.10) and the criterion (5.3) may be used to obtain the solution of the original equation (1.1) up to $t < t_*$. For small β the time t_* is very long as is clear from Fig. 5.6. When one considers the smallness of β one should consider actually the smallness of βe^2 due to the exponential proliferation of the number of terms (see Eq. 4.6 of [46]).

Assuming that the Q'_n give a good approximaion of the Q_n for $t < t_*$, we can use Fig. 5.7 to conclude that, for example, for $\beta = 0.1$ our solution is meaningful up to time $t = 10^{4.3}$ and therefore can be whithin reach of works like [43, 44]. The assumption obove corresponds to the observation that correcting c_4 and c_9 by Q_4 and Q_9 is not changed much over time, and therefore all the Q'_n stay small for a very long time. Note, that since the largest localization length for $W = 4$ is approximatelly 6, positions 4 and 9 are within one localization length from the initial data. Therefore their removal does not affect the behavior for large n that is relevant for the asymptotics.

Additional benifit of this implemamtnation is the computational speed. For example, even for the 3rd order of the pertrurbation theory one can compute the perturbative solution up to $t < 10^4$ in 10 minutes while using the same computer an exact convergent integration (split-step method) takes 28 hours, which is a two orders of magnitude speed-up.

6. Summary and Discussion

In this paper we have demonstrated how a perturbation theory can be numerically implemented for the solution of the NLSE with a random potential (1.1). In the perturbative method the computer is used to implement the symbolic recursive calculation of the various terms and also for their numerical evaluation. This method allows to estimate the errors since the remainder term is bounded. It was demonstrated (in the end of the previous section) how evaluate the time of validity of the perturbation theory. This approach has also a great advantage in the speed of the calculation. We believe that the method can be generalized to other nonlinear differential equations, for example, the Fermi-Ulam-Pasta problem.

In order to make the perturbation theory of a much greater value one has to solve the problem of resonant terms (when R_n^{-1} of (5.2) is large). In other words the degenerate perturbation theory should be extended to nonlinear equations. Also the asymptotic nature of the perturbation theory is not known, it is not clear when it is convergent and when only asymptotic.

We enjoyed many extensive illuminating and extremely critical discussions with Michael Aizenman. We also had informative discussions with S. Aubry, V. Chulaevski, S. Flach, I. Goldshield, M. Goldstein, I. Guarneri, M. Sieber, W.-M. Wang and S. Warzel. This work was partly supported by the Israel Science Foundation (ISF), by the US-Israel Binational Science Foundation (BSF), by the USA National Science Foundation (NSF DMS-0903651), by the Minerva Center of Nonlinear Physics of Complex Systems, by the Shlomo Kaplansky academic chair, by the Fund for promotion of research at the Technion and by the E. and J. Bishop research fund.

Appendix

In the calculations of the paper we used the expansion (2.10) of the wavefunction and the expansion coefficients $c_n(t)$ are calculated from (2.6) and (2.13). The $c_n^{(l)}(t)$ depend on β since the $E_n^{'}$ in (2.13) depend on it. Therefore (2.6) is not a Taylor series in β. In this Appendix it is shown that this expansion is equivalent to the Taylor series,

$$c_n = \sum_{l=0}^{\infty} \bar{c}_n^{(l)} \beta^l.$$

Contrary to the $c_n^{(l)}$ the $\bar{c}_n^{(l)}$ are independent of β. The expansion of (2.12) in powers of β produces the following equation for the r-th order

(6.1)

$$i\partial_t \bar{c}_n^{(r)} = -\sum_{l=1}^{r}\sum_{l_1=0}^{l} \frac{1}{l_1!}\left(\frac{\partial^{l_1} E_n^{(l-l_1)}}{\partial \beta^{l_1}}\right)_{\beta=0} \bar{c}_n^{(r-l)} + \\ + \sum_{\sum_i l_i = r-1} \sum_{\{m_i\}} V_n^{m_1 m_2 m_3} \bar{c}_{m_1}^{*(l_1)} \bar{c}_{m_2}^{(l_2)} \bar{c}_{m_3}^{(l_3)} \left(\frac{1}{l_4!}\frac{\partial^{l_4}}{\partial \beta^{l_4}} e^{i\left(E_n' + E_{m_1}' - E_{m_2}' - E_{m_3}'\right)t}\right)_{\beta=0}.$$

We considered a different expansion (2.13), where one does not expand the exponent, but still compares the implicit powers of β from both sides of the equation. The equation for the $(r-k)$ order in this expansion is (that is just (2.13))

(6.2)

$$i\partial_t c_n^{(r-k)} = -\sum_{l=1}^{r-k} E_n^{(l)} c_n^{(r-k-l)} \\ + \sum_{\{m_i\}} \sum_{l_1+l_2+l_3=r-k-1} V_n^{m_1 m_2 m_3} c_{m_1}^{*(l_1)} c_{m_2}^{(l_2)} c_{m_3}^{(l_3)} e^{i\left(E_n' + E_{m_1}' - E_{m_2}' - E_{m_3}'\right)t}.$$

It can be shown that each term in this expansion is uniformly bounded in time, with a proper selection of E_n', that is the secular terms are removed. We will show that this expansion is equivalent to a Taylor series.

Theorem 1. *For any t,*

$$c_n = \sum_{k=0}^{\infty} c_n^{(k)} \beta^k, \tag{6.3}$$

where $c_n^{(k)}$ are defined using (6.2).

Proof. Since $c_n = \sum_{k=0}^{\infty} \bar{c}_n^{(k)} \beta^k$ is the expansion of c_n in powers of β, and due to the uniqueness of this expansion, the theorem is true if and only if

$$\bar{c}_n^{(r)} = \sum_{k=0}^{r} \frac{1}{k!}\left(\frac{\partial^k c_n^{(r-k)}}{\partial \beta^k}\right)_{\beta=0} = \sum_{k=0}^{r-1} \frac{1}{k!}\left(\frac{\partial^k c_n^{(r-k)}}{\partial \beta^k}\right)_{\beta=0}, \tag{6.4}$$

where at the last equality we have used the fact that $\frac{\partial^r c_n^{(0)}}{\partial \beta^r} = 0$, for any $r \geq 1$. We proceed to prove this equality by induction. Suppose that this equality is true for

all the orders till order r. We apply the linear operator $\sum_{k=0}^{r-1} \frac{1}{k!}\frac{\partial^k}{\partial\beta^k}$ to both sides of (6.2). For the first part on the RHS we get

$$\sum_{k=0}^{r-1}\frac{1}{k!}\sum_{l=1}^{r-k}\frac{\partial^k}{\partial\beta^k}\left(E_n^{(l)}c_n^{(r-k-l)}\right) =$$

$$= \sum_{k=0}^{r-1}\frac{1}{k!}\sum_{l=1}^{r-k}\sum_{l_1=0}^{k}\frac{k!}{l_1!\,(k-l_1)!}\frac{\partial^{l_1}E_n^{(l)}}{\partial\beta^{l_1}}\frac{\partial^{(k-l_1)}c_n^{(r-k-l)}}{\partial\beta^{(k-l_1)}}$$

$$= \sum_{k=0}^{r-1}\sum_{l=1}^{r-k}\sum_{l_1=0}^{k}\left(\frac{1}{l_1!}\frac{\partial^{l_1}E_n^{(l)}}{\partial\beta^{l_1}}\right)\left(\frac{1}{(k-l_1)!}\frac{\partial^{(k-l_1)}c_n^{(r-k-l)}}{\partial\beta^{(k-l_1)}}\right) \tag{6.5}$$

where at the first equality we have used the Leibniz generalized product rule. We now exchange variables such that

$$\begin{aligned} l_1 &= l_1 \\ l_2 &= k - l_1 \\ z &= l + l_1 \end{aligned} \tag{6.6}$$

or in a matrix notation

$$\begin{pmatrix} l_1 \\ l_2 \\ z \end{pmatrix} = A_1 \begin{pmatrix} l_1 \\ l \\ k \end{pmatrix}, \tag{6.7}$$

where

$$A_1 = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}.$$

The region of summation is bounded by the planes

$$\begin{aligned} 0 &\leq k \leq r-1 \\ 1 &\leq l \leq r-k \\ 0 &\leq l_1 \leq k \end{aligned} \tag{6.8}$$

or in matrix notation

$$B_1 \begin{pmatrix} l_1 \\ l \\ k \end{pmatrix} \leq \begin{pmatrix} r-1 \\ r \\ 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \tag{6.9}$$

where

$$B_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Changing the variables by applying the transformation matrix produces

$$B_1 \cdot A_1^{-1} \begin{pmatrix} l_1 \\ l_2 \\ z \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \end{pmatrix} \begin{pmatrix} l_1 \\ l_2 \\ z \end{pmatrix} \leq \begin{pmatrix} r-1 \\ r \\ 0 \\ 0 \\ -1 \\ 0 \end{pmatrix} \tag{6.10}$$

or the following inequalities

$$\begin{aligned} l_1 + l_2 &\leq r-1 \\ l_2 + z &\leq r \\ 0 &\leq l_2 \\ 0 &\leq l_1 \\ l_1 &\leq z-1 \\ 0 &\leq l_1 + l_2. \end{aligned} \tag{6.11}$$

Removing redundant inequalities gives

$$\begin{aligned} 0 \leq l_1 &\leq z-1 \\ 1 &\leq z \leq r \\ 0 &\leq l_2 \leq r-z. \end{aligned} \tag{6.12}$$

Therefore in the new variables the sum (6.5) takes the form

$$\sum_{z=1}^{r} \sum_{l_1=0}^{z-1} \sum_{l_2=0}^{r-z} \left(\frac{1}{l_1!} \frac{\partial^{l_1} E_n^{(z-l_1)}}{\partial \beta^{l_1}} \right) \left(\frac{1}{l_2!} \frac{\partial^{l_2} c_n^{(r-z-l_2)}}{\partial \beta^{l_2}} \right), \tag{6.13}$$

Since $\frac{\partial^z E_n^{(0)}}{\partial \beta^z} = 0$ for any $z \geq 1$,we can write

$$\sum_{z=1}^{r} \sum_{l_1=0}^{z} \sum_{l_2=0}^{r-z} \left(\frac{1}{l_1!} \frac{\partial^{l_1} E_n^{(z-l_1)}}{\partial \beta^{l_1}} \right) \left(\frac{1}{l_2!} \frac{\partial^{l_2} c_n^{(r-z-l_2)}}{\partial \beta^{l_2}} \right). \tag{6.14}$$

Taking $\beta = 0$ and using the assumption of the induction for orders lower than r we have

$$\sum_{z=1}^{r} \sum_{l_1=0}^{z} \left(\frac{1}{l_1!} \frac{\partial^{l_1} E_n^{(z-l_1)}}{\partial \beta^{l_1}} \right) \bar{c}_n^{(r-z)}, \tag{6.15}$$

which is the first expression for $i\partial_t \bar{c}_n^{(r)}$. The proof for the second term is similar, operating with $\sum_{k=0}^{r-1} \frac{1}{k!} \frac{\partial^k}{\partial \beta^k}$ on the second term in (6.2) gives

$$\sum_{\{m_i\}} V_n^{m_1 m_2 m_3} \sum_{k=0}^{r-1} \sum_{l_1=0}^{r-k-1} \sum_{l_2=0}^{r-k-1-l_1} \frac{1}{k!} \frac{\partial^k}{\partial \beta^k} \left(c_{m_1}^{*(l_1)} c_{m_2}^{(l_2)} c_{m_3}^{(r-k-1-l_1-l_2)} e^{i\left(E'_n + E'_{m_1} - E'_{m_2} - E'_{m_3}\right)t} \right). \tag{6.16}$$

Using the Leibniz generalized product rule, which states

$$\frac{\partial^k}{\partial \beta^k} (x_1 x_2 x_3 x_4) = \sum_{s_1+s_2+s_3+s_4=k} \frac{k!}{s_1! s_2! s_3! s_4!} \frac{\partial^{s_1} x_1}{\partial \beta^{s_1}} \frac{\partial^{s_2} x_2}{\partial \beta^{s_2}} \frac{\partial^{s_3} x_3}{\partial \beta^{s_3}} \frac{\partial^{s_4} x_4}{\partial \beta^{s_4}} \tag{6.17}$$

we have the sum

$$\sum_{\{m_i\}} V_n^{m_1 m_2 m_3} \sum_{k=0}^{r-1} \sum_{l_1=0}^{r-k-1} \sum_{l_2=0}^{r-k-1-l_1} \sum_{s_1=0}^{k} \sum_{s_2=0}^{k-s_1} \sum_{s_3=0}^{k-s_1-s_2} \left(\frac{1}{s_1!} \frac{\partial^{s_1} c_{m_1}^{*(l_1)}}{\partial \beta^{s_1}} \right) \left(\frac{1}{s_2!} \frac{\partial^{s_2} c_{m_2}^{(l_2)}}{\partial \beta^{s_2}} \right) \times \tag{6.18}$$
$$\times \left(\frac{1}{s_3!} \frac{\partial^{s_3} c_{m_3}^{(r-k-1-l_1-l_2)}}{\partial \beta^{s_3}} \right) \left(\frac{1}{(k-s_1-s_2-s_3)!} \frac{\partial^{(k-s_1-s_2-s_3)}}{\partial \beta^{(k-s_1-s_2-s_3)}} e^{i\left(E'_n + E'_{m_1} - E'_{m_2} - E'_{m_3}\right)t} \right)$$

Following the first part of this proof we exchange the variable to

$$\begin{aligned} z_1 &= l_1 + s_1 \\ z_2 &= l_2 + s_2 \\ z_3 &= k - s_1 - s_2 - s_3 \\ s_i &= s_i \end{aligned} \tag{6.19}$$

or using a transformation matrix

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ s_1 \\ s_2 \\ s_3 \end{pmatrix} = A_2 \begin{pmatrix} k \\ l_1 \\ l_2 \\ s_1 \\ s_2 \\ s_3 \end{pmatrix}, \tag{6.20}$$

where

$$A_2 = \begin{pmatrix} 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & -1 & -1 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The region of summation is bounded by the following hyperplanes

$$\begin{aligned} 0 &\leq k \leq r-1 \\ 0 &\leq l_1 \leq r-k-1 \\ 0 &\leq l_2 \leq r-k-1-l_1 \\ 0 &\leq s_1 \leq k \\ 0 &\leq s_2 \leq k-s_1 \\ 0 &\leq s_3 \leq k-s_1-s_2 \end{aligned} \tag{6.21}$$

which could be represented in a matrix notation as

$$B_2 \begin{pmatrix} k \\ l_1 \\ l_2 \\ s_1 \\ s_2 \\ s_3 \end{pmatrix} \leq \begin{pmatrix} r-1 \\ r-1 \\ r-1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{6.22}$$

where

$$B_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 & 1 & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

Using the transformation matrix to change the variables results in the following

$$\begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & -1 & -1 \\ 0 & 0 & -1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & -1 & -1 \\ -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ s_1 \\ s_2 \\ s_3 \end{pmatrix} \leq \begin{pmatrix} r-1 \\ r-1 \\ r-1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{6.23}$$

or in the following inequalities

$$
\begin{aligned}
z_3 + s_1 + s_2 + s_3 &\leq r-1 \\
z_1 + z_3 + s_2 + s_3 &\leq r-1 \\
z_1 + z_2 + z_3 + s_3 &\leq r-1 \\
0 &\leq z_3 + s_2 + s_3 \\
0 &\leq z_3 + s_3 \\
0 &\leq z_3 \\
0 &\leq z_3 + s_1 + s_2 + s_3 \\
s_1 &\leq z_1 \\
s_2 &\leq z_2 \\
0 &\leq s_i
\end{aligned}
\tag{6.24}
$$

Removing redundant inequalities gives

$$
\begin{aligned}
0 &\leq s_1 \leq z_1 \\
0 &\leq s_2 \leq z_2 \\
0 &\leq s_3 \leq (r-1) - z_1 - z_2 - z_3 \\
0 &\leq z_1 \leq (r-1) - z_3 \\
0 &\leq z_2 \leq (r-1) - z_1 - z_3 \\
0 &\leq z_3 \leq r-1
\end{aligned}
\tag{6.25}
$$

which is equivalent to the sum

$$
\sum_{\{m_i\}} V_n^{m_1 m_2 m_3} \sum_{z_3=0}^{r-1} \sum_{z_1=0}^{r-1-z_3} \sum_{z_2=0}^{r-1-z_1-z_3} \sum_{s_1=0}^{z_1} \sum_{s_2=0}^{z_2} \sum_{s_3=0}^{r-1-z_1-z_2-z_3} \left(\frac{1}{s_1!} \frac{\partial^{s_1} c_{m_1}^{*(z_1-s_1)}}{\partial \beta^{s_1}} \right) \times
$$

$$
\times \left(\frac{1}{s_2!} \frac{\partial^{s_2} c_{m_2}^{(z_2-s_2)}}{\partial \beta^{s_2}} \right) \left(\frac{1}{s_3!} \frac{\partial^{s_3} c_{m_3}^{(r-1-z_1-z_2-z_3-s_3)}}{\partial \beta^{s_3}} \right) \left(\frac{1}{z_3!} \frac{\partial^{z_3}}{\partial \beta^{z_3}} e^{i\left(E'_n + E'_{m_1} - E'_{m_2} - E'_{m_3}\right)t} \right) \tag{6.26}
$$

Putting $\beta = 0$ and utilizing the assumption of the induction we get

$$
\sum_{l_1+l_2+l_3+l_4=r-1} \sum_{\{m_i\}} V_n^{m_1 m_2 m_3} \bar{c}_{m_1}^{(l_1)*} \bar{c}_{m_2}^{(l_2)} \bar{c}_{m_3}^{(l_3)} \left(\frac{1}{l_4!} \frac{\partial^{l_4}}{\partial \beta^{l_4}} e^{i\left(E'_n + E'_{m_1} - E'_{m_2} - E'_{m_3}\right)t} \right)_{\beta=0} \tag{6.27}
$$

which is exactly the second term in the equation for $i\partial_t \bar{c}_n^{(r)}$. Since the zero order trivially satisfies this theorem, this competes the proof by induction. □

One should be able to extend the results of this Appendix to other nonlinear equations, for example, where the power of the nonlinearity is different (in the last term of (1.1) 2 is replaced by another integer).

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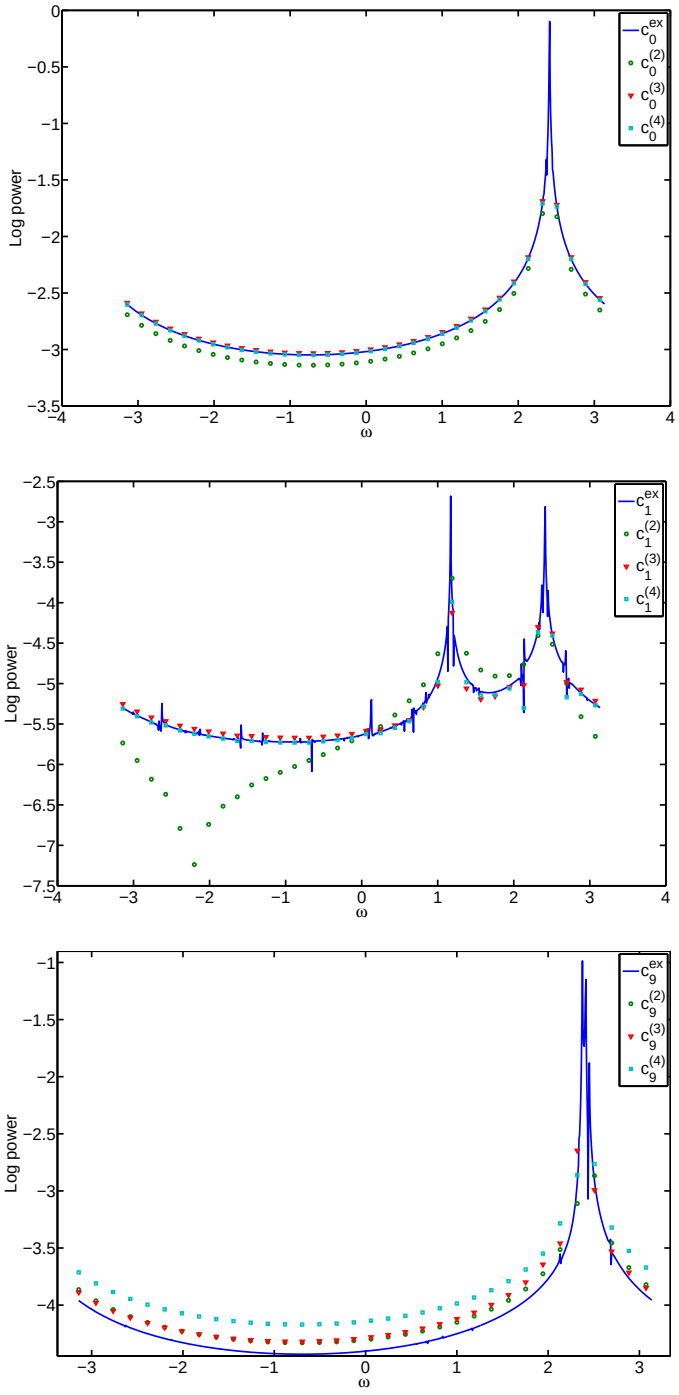

Figure 5.1: Fourier transform of $\bar{c}_0$, $\bar{c}_1$ and $\bar{c}_9$ for different orders of the perturbation theory compared to the Fourier transform of an exact solution, c_n, (solid line). Second order is given by green crosses, third order by red triangles and fourth order by blue squares. The parameters are: $\beta = 0.0774$, $t = 1000$, $W = 4$, $J = 1$.